

Electronic Supplementary Information: part 3

Photoactivatable HNO-releasing Compounds Using the retro-Diels-Alder Reaction

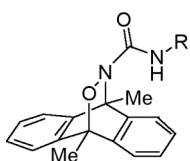
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<NMR charts>

Contents



- 1:** R = 4-nitrophenyl
- 2:** R = H
- 3:** R = 4-nitrobenzyl
- 4:** R = 3-nitrophenyl
- 5:** R = 4'-nitrobiphenyl
- 6:** R = 4'-nitrostyryl

Chart S3-1: Compound **1**, ¹H-NMR

Chart S3-2: Compound **1**, ¹³C-NMR

Chart S3-3: Compound **2**, ¹H-NMR

Chart S3-4: Compound **2**, ¹³C-NMR

Chart S3-5: Compound **3**, ¹H-NMR

Chart S3-6: Compound **3**, ¹³C-NMR

Chart S3-7: Compound **4**, ¹H-NMR

Chart S3-8: Compound **4**, ¹³C-NMR

Chart S3-9: Compound **5**, ¹H-NMR

Chart S3-10: Compound **5**, ¹³C-NMR-1 (accumulation for 2 hr)

Chart S3-11: Compound **5**, ¹³C-NMR-2 (accumulation for 13 hr 45 min). Due to the long time accumulation need to identify quaternary carbon atoms of the compound, the carbon signals attributed to the thermal decomposition products, 4-(4'-nitrophenyl)aniline and 9,10-dimethylanthracene, appeared in this charts even under the isothermal control (at 20°C for DMSO-d₆ solvent). These thermal decomposition products were substantially not observed in the chart accumulated for 2 hr (Chart S3-10).

Chart S3-12: Compound **6**, ¹H-NMR

Chart S3-1

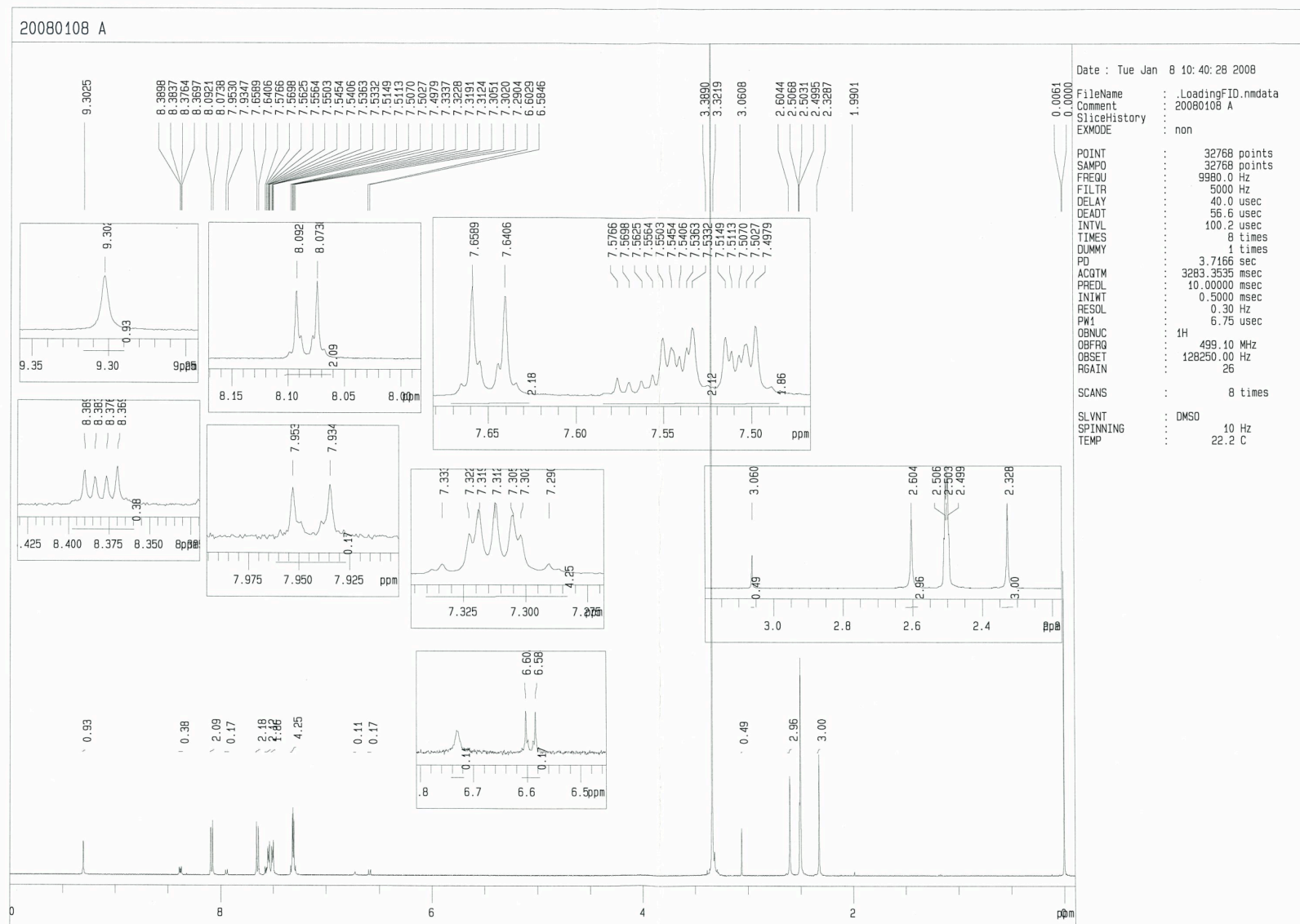
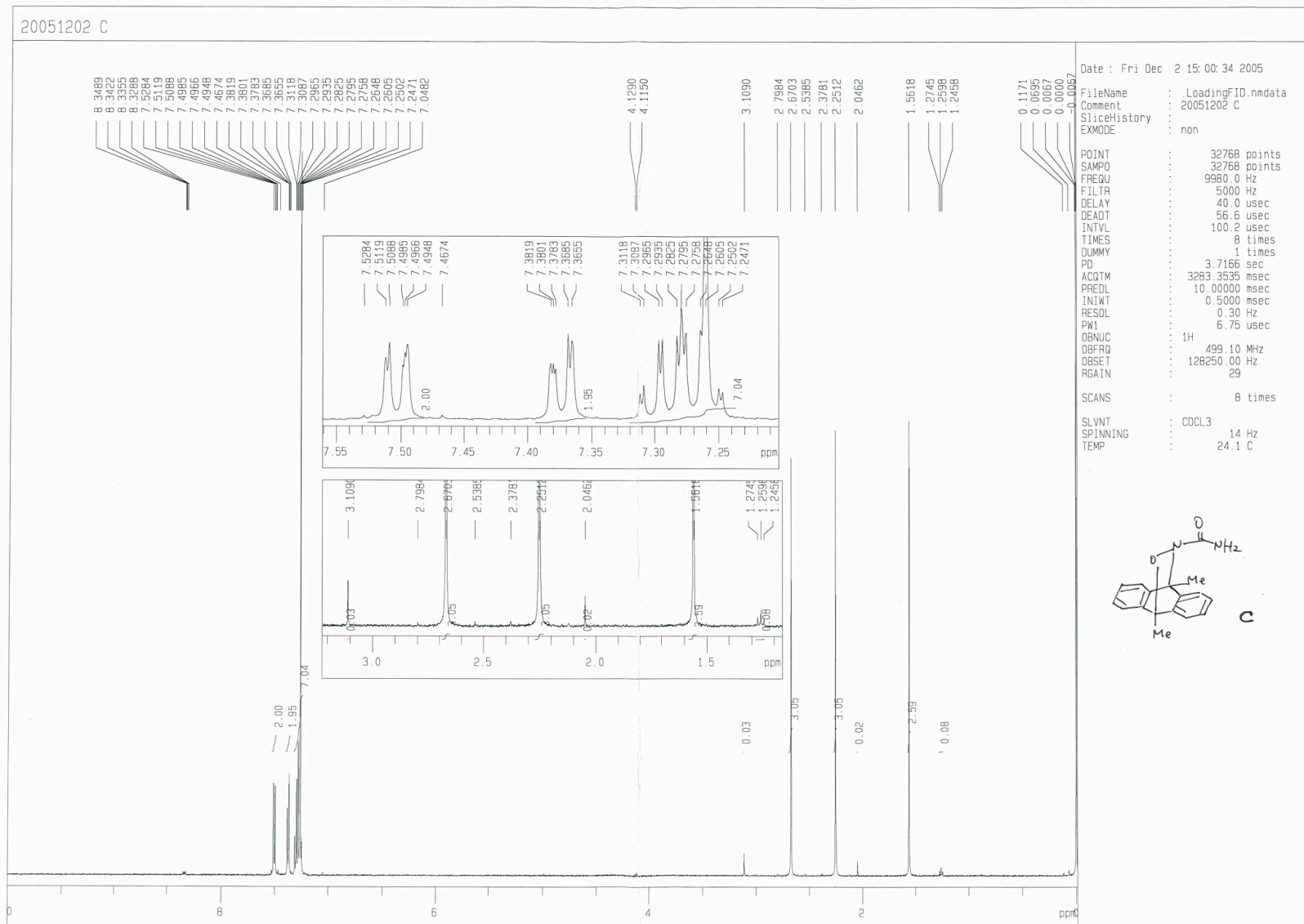




Chart S3-3



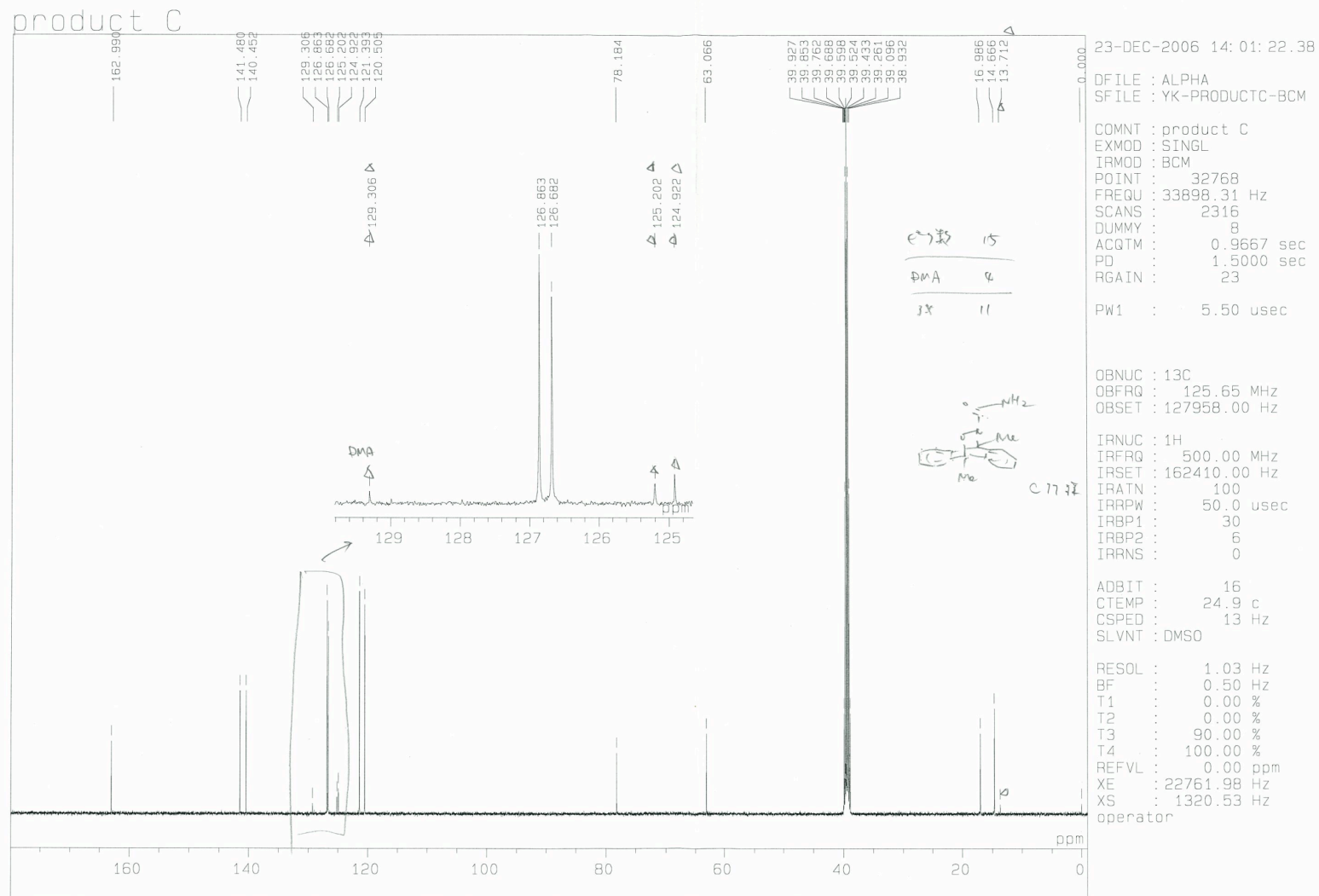
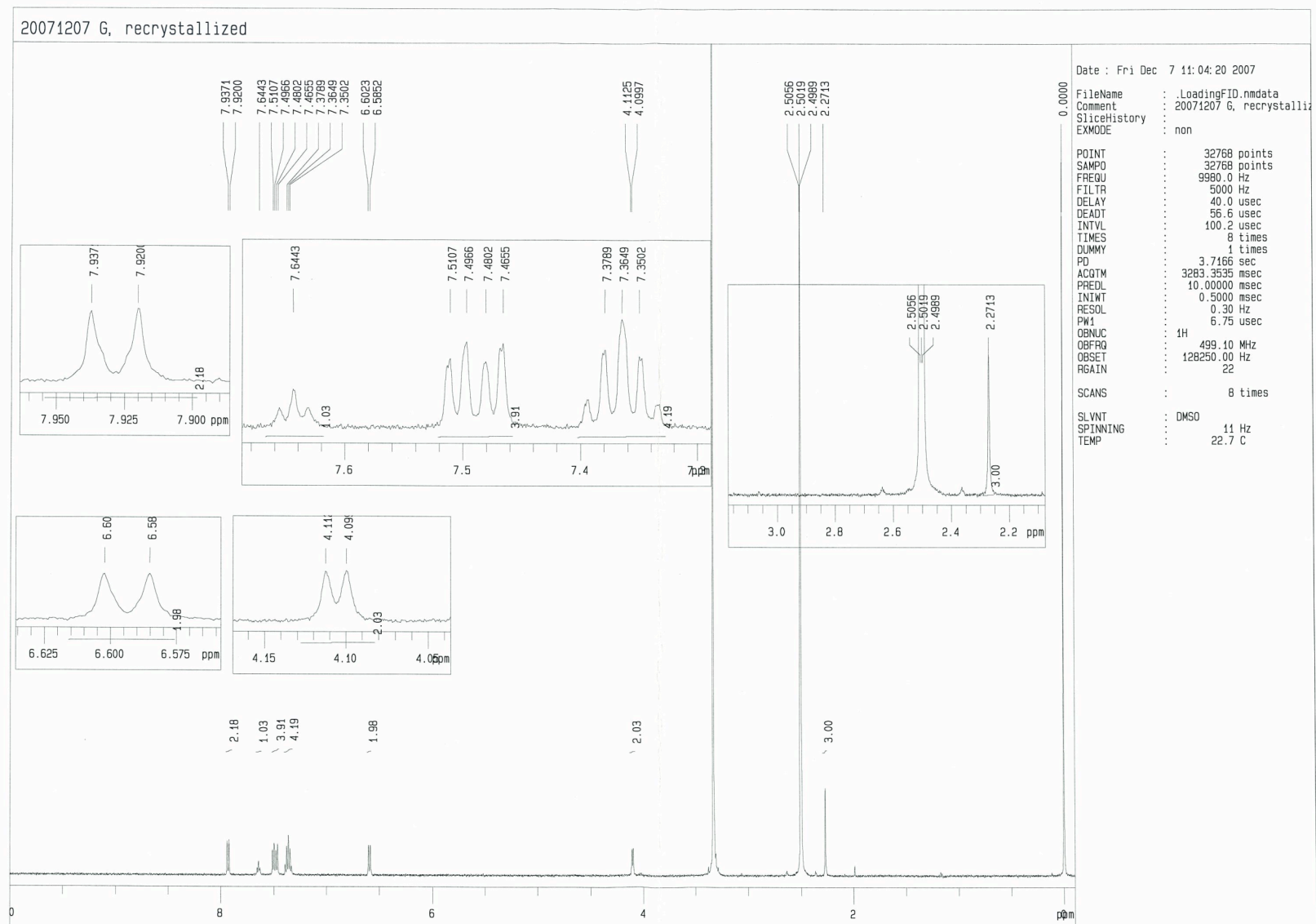


Chart S3-4

Chart S3-5



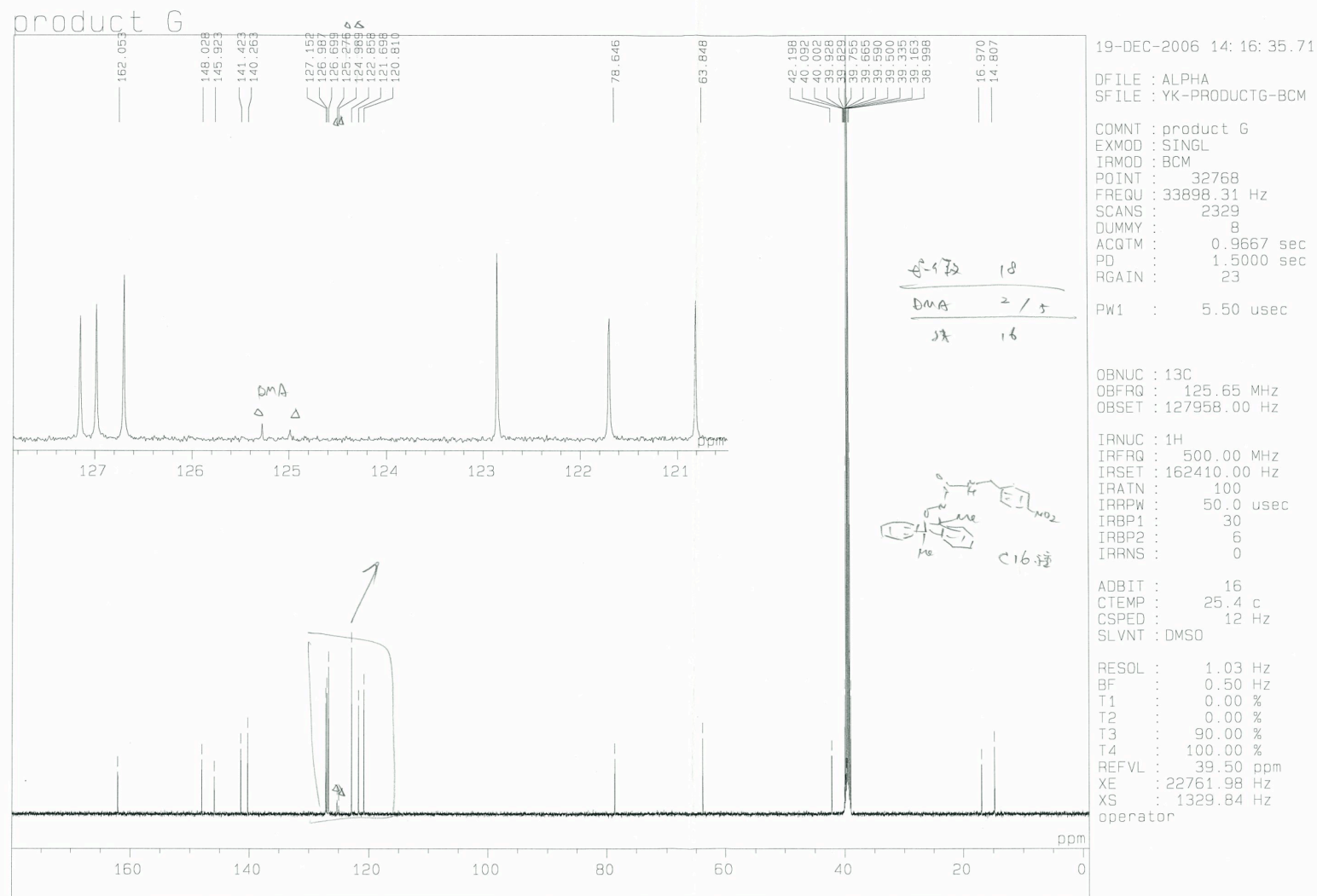
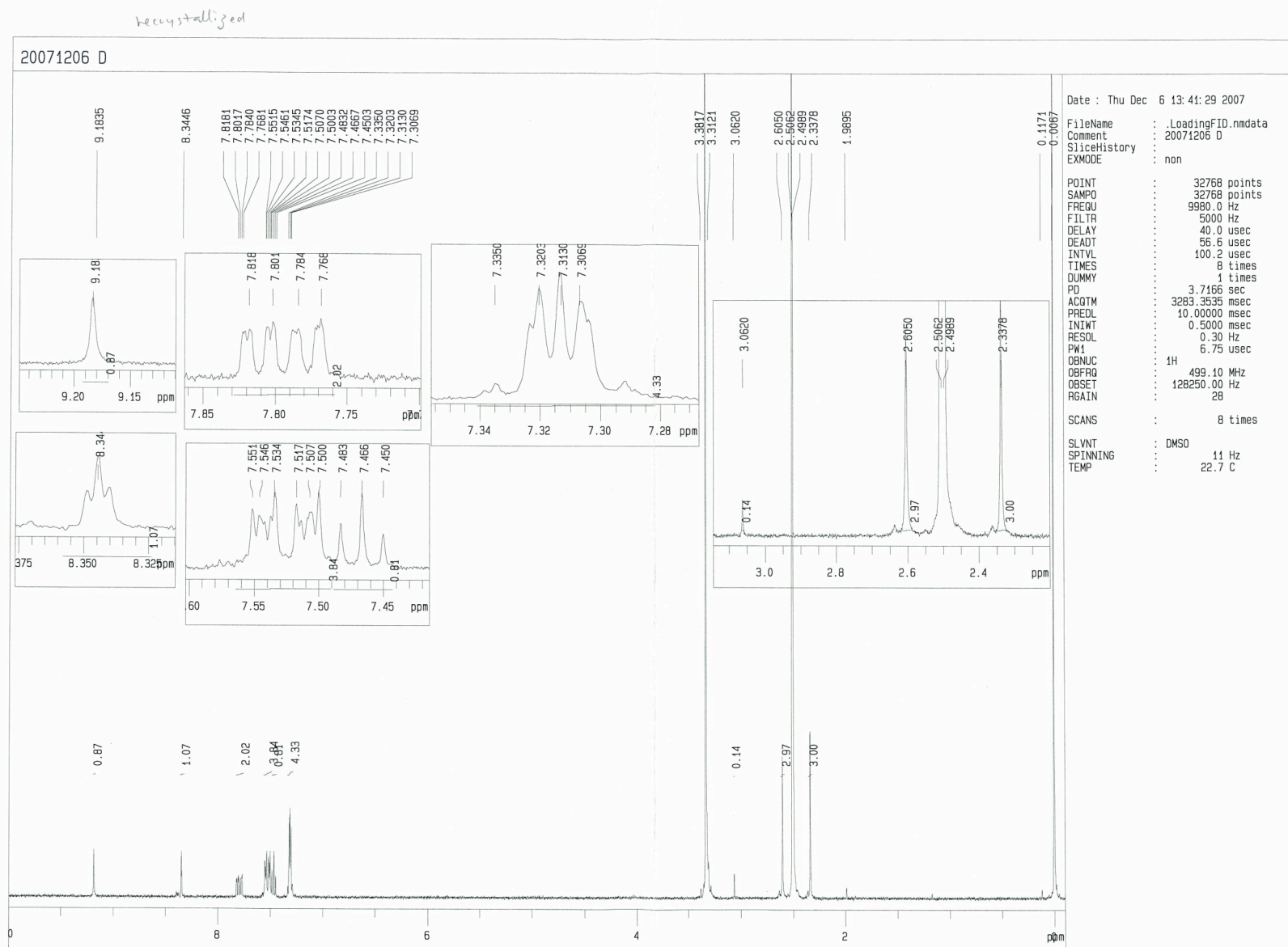


Chart S3-6

Chart S3-7



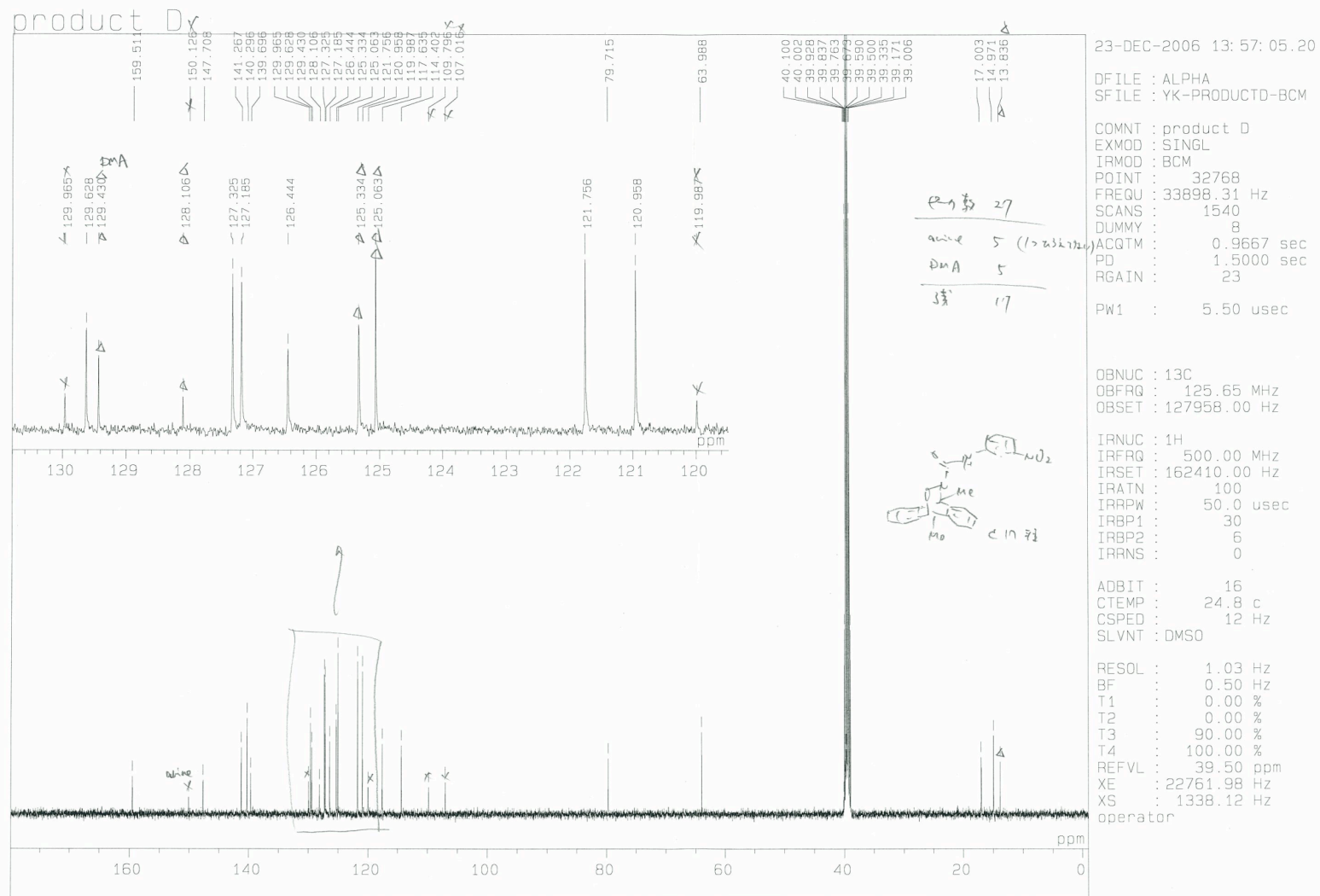
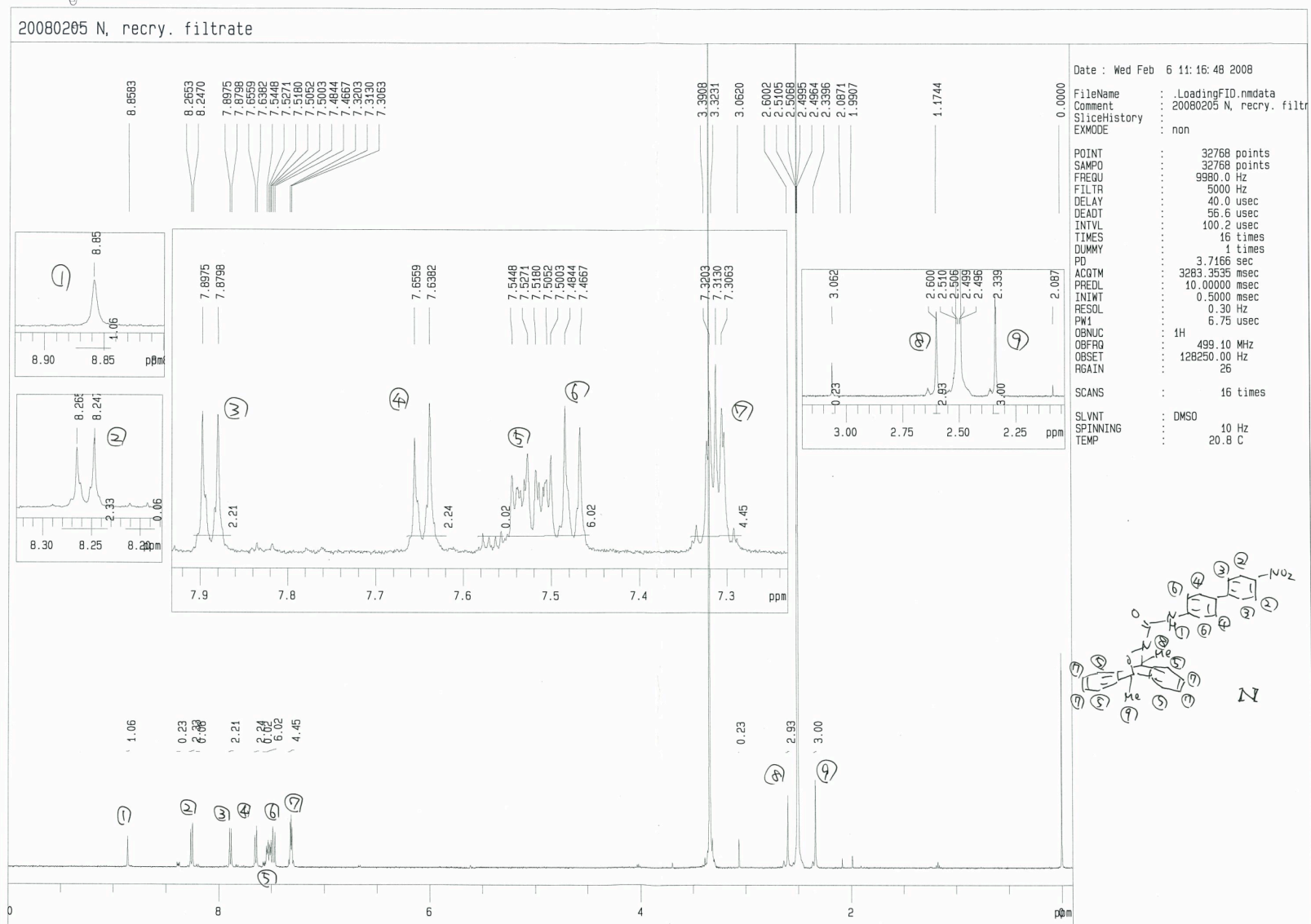
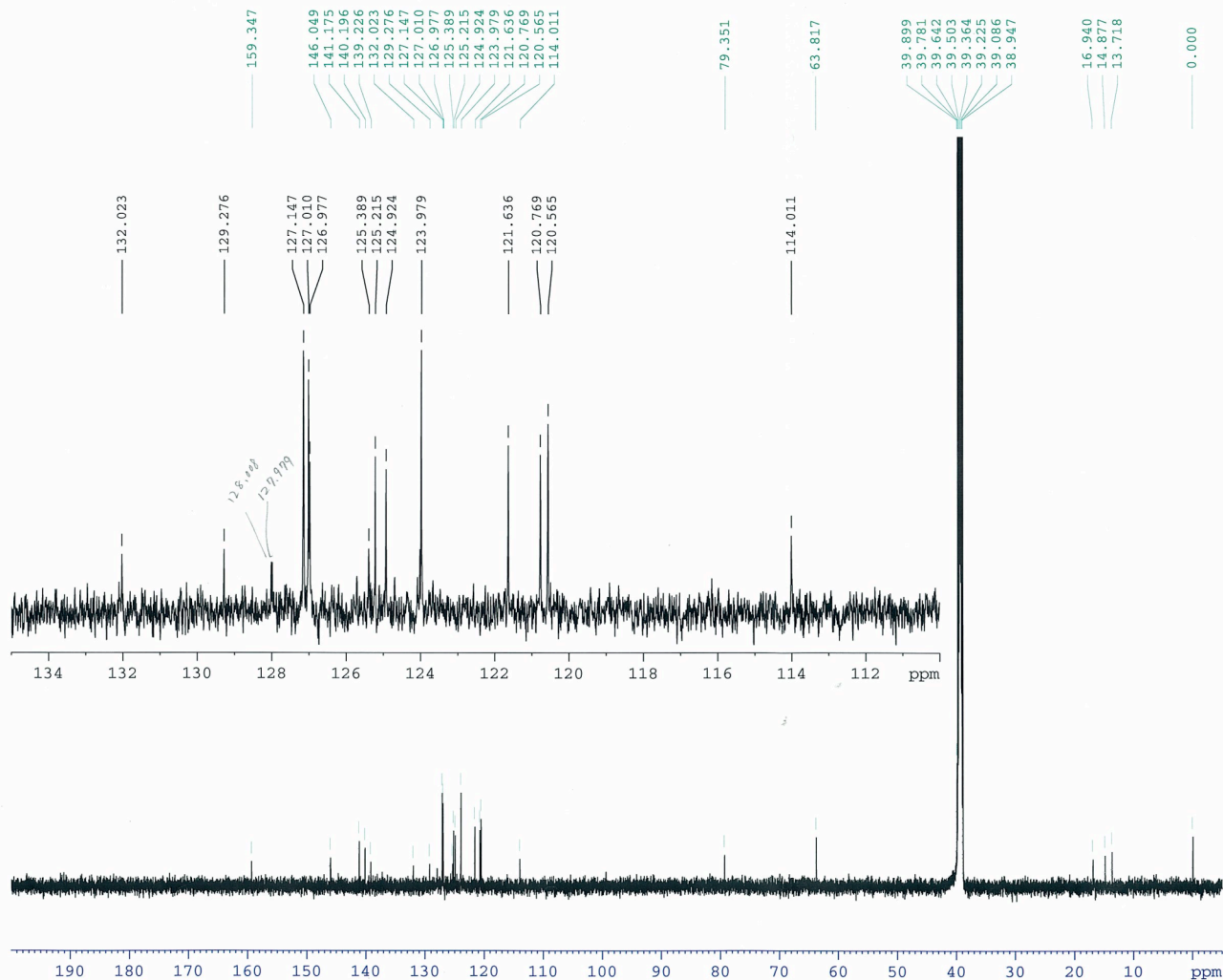


Chart S3-9



product N/carbon



Current Data Parameters
NAME yk_matsuo
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080512
Time 10.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2873
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9110143 sec
RG 20642.5
DW 13.900 usec
DE 25.00 usec
TE 293.0 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.00 usec
PL1 1.00 dB
SFO1 150.9178988 MHz

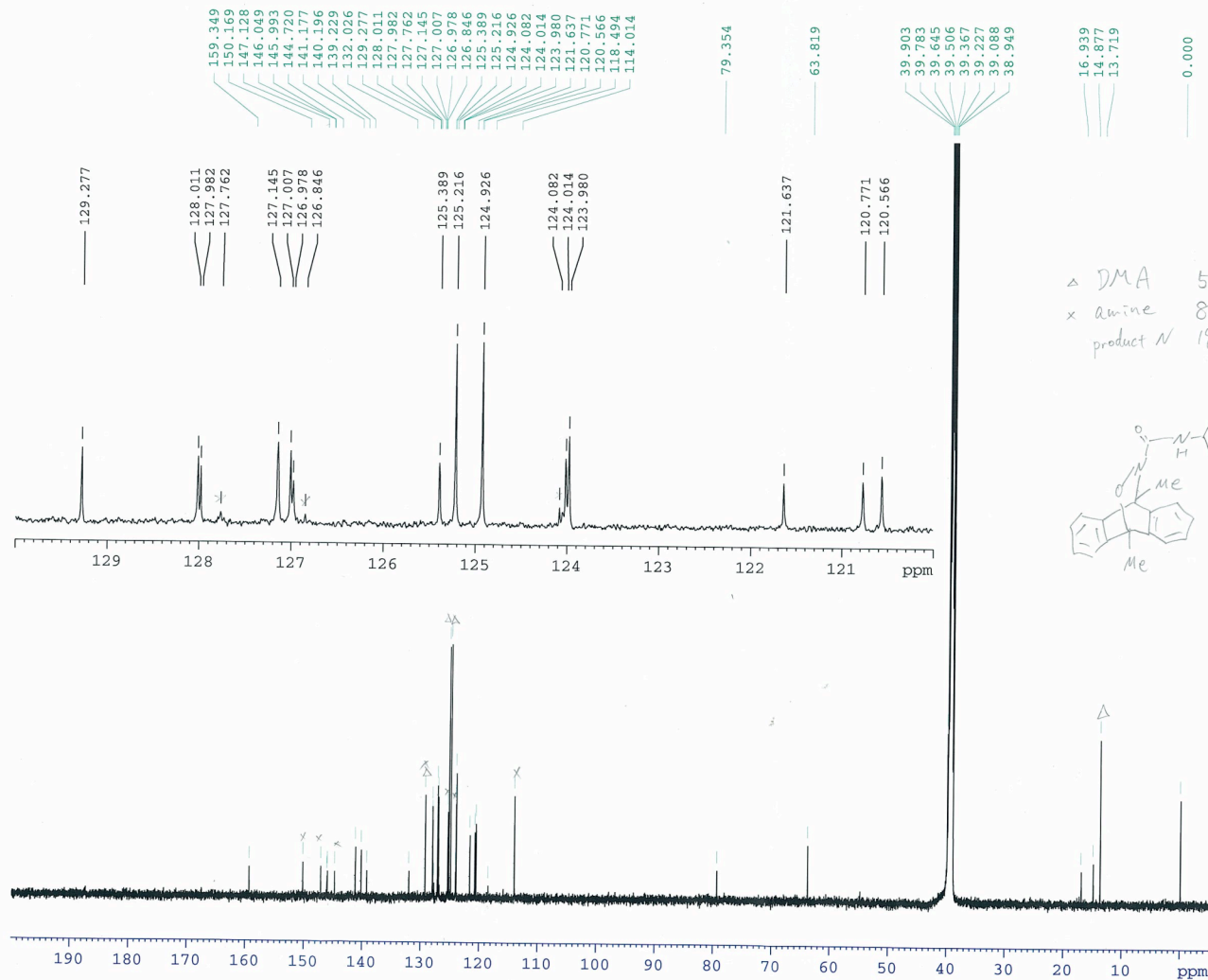
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CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 600.1324005 MHz

F1 - Acquisition parameters
ND0 2
TD 128
SFO1 600.1333 MHz
FIDRES 44.796444 Hz
SW 9.554 ppm
FMODE QF

F2 - Processing parameters
SI 32768
SF 150.9028962 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 1024
MC2 QF
SF 600.1300047 MHz
WDW nc
SSB 0
LB 0.30 Hz
GB 0.1

product N/carbon



Current Data Parameters
NAME yk_matsuo
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080513
Time 4.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 35971.223 Hz
FIDRES 0.548877 Hz
AQ 0.9110143 sec
RG 20642.5
DW 13.900 usec
DE 25.00 usec
TE 293.0 K
D1 1.50000000 sec
d11 0.03000000 sec
DELTA 1.39999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

===== CHANNEL f1 =====
NUC1 13C
P1 4.00 usec
PL1 -1.00 dB
SFO1 150.9178988 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -6.00 dB
PL12 12.00 dB
PL13 12.00 dB
SFO2 600.1324005 MHz

F2 - Processing parameters
SI 32768
SF 150.9028959 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

